

chain nodes :
7 8 9 10 11 12 18 27 28 29 31
ring nodes :
1 2 3 4 5 6 21 22 23 24 25 26
chain bonds :
6-8 7-23 8-18 10-11 11-12 18-28 26-27 27-29
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 21-22 21-26 22-23 23-24 24-25 25-26
exact/norm bonds :
6-8 7-23 8-18 18-28 26-27 27-29
exact bonds :
10-11 11-12 21-22 21-26 22-23 23-24 24-25 25-26
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 21 :

G1:[*1-*2],[*3-*4]

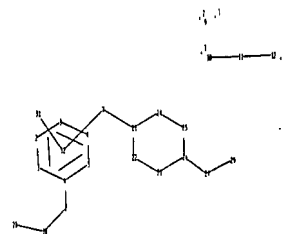
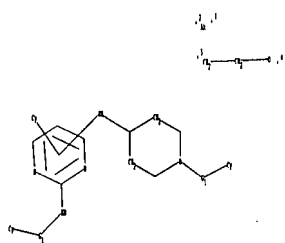
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS12:CLASS18:CLASS
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS28:Atom 29:Atom 31:Atom 32:Atom
Generic attributes :
28:
Saturation : Unsaturated
29:

Saturation : Unsaturated
31:
Saturation : Unsaturated

10/517,594

=>

Uploading C:\Program Files\Stnexp\Queries\10517594.str



chain nodes :

7 8 9 10 11 12 18 27 28 29 31

ring nodes :

1 2 3 4 5 6 21 22 23 24 25 26

chain bonds :

6-8 7-23 8-18 10-11 11-12 18-28 26-27 27-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 21-22 21-26 22-23 23-24 24-25 25-26

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6-8 7-23 8-18 18-28 26-27 27-29

exact bonds :

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normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 21 :

G1:[*1-*2],[*3-*4]

Match level.:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 18:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:CLASS 28:Atom 29:Atom 31:Atom 32:Atom

Generic attributes :

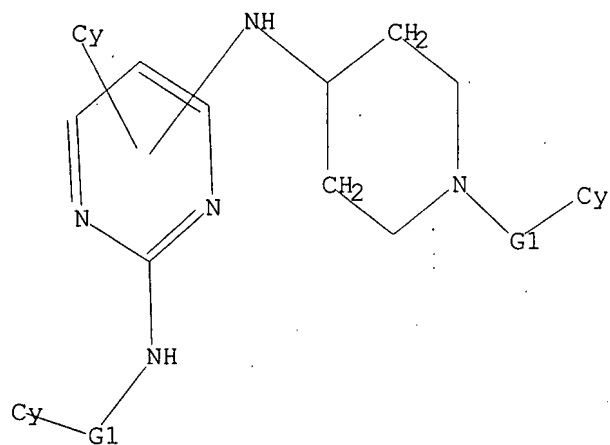
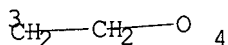
10/517,594

28:
Saturation : Unsaturated
29:
Saturation : Unsaturated
31:
Saturation : Unsaturated

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

Ak¹



G1 [01-02],[03-04]

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
SAMPLE SEARCH INITIATED 16:33:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 6392 TO ITERATE

31.3% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

10/517,594

PROJECTED ITERATIONS: 123047 TO 132633
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss ful
FULL SEARCH INITIATED 16:33:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 130540 TO ITERATE

100.0% PROCESSED 130540 ITERATIONS
SEARCH TIME: 00.00.04

24 ANSWERS

L3 24 SEA SSS FUL L1

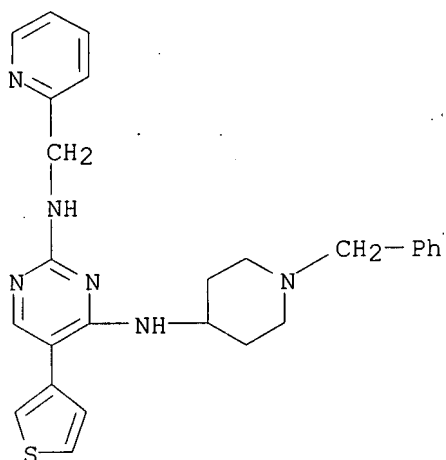
=> => s l3
L4 1 L3

=> d 14 bib,ab,hitstr

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
 AN 2003:1006977 CAPLUS
 DN 140:59654
 TI Preparation of substituted diaminopyrimidines as protein kinase C θ inhibitors
 IN Baudler, Monika; Bhagwat, Shripad S.; Erdman, Paul E.; Baudler, Monika; Bhagwat, Shripad S.; Erdman, Paul E.; Gantner, Florian; Palanki, Moorthy S. S.; Schudt, Christian; Stadlwieser, Josef; Zapf, James
 PA Altana Pharma A.-G., Germany; Signal Pharmaceuticals, Inc.
 SO PCT Int. Appl., 42 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

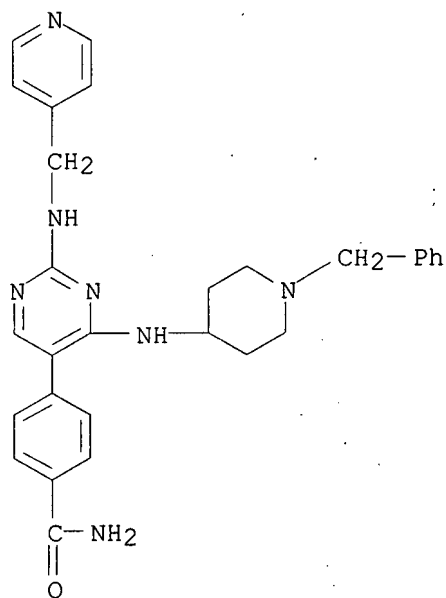
Appl.

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|--|------|----------|-----------------|----------|
| PI | WO 2003106451 | A1 | 20031224 | WO 2003-EP6016 | 20030607 |
| | W: AE, AL, AU, BA, BR, CA, CN, CO, CU, DZ, EC, GE, HR, ID, IL, IN, IS, JP, KR, LT, LV, MA, MK, MX, NO, NZ, PH, PL, SG, TN, UA, US, VN, YU, ZA, ZW | | | | |
| | RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR | | | | |
| | CA 2489458 | A1 | 20031224 | CA 2003-2489458 | 20030607 |
| | AU 2003236720 | A1 | 20031231 | AU 2003-236720 | 20030607 |
| | EP 1515964 | A1 | 20050323 | EP 2003-735581 | 20030607 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| | US 2005222186 | A1 | 20051006 | US 2004-517594 | 20041213 |
| PRAI | US 2002-388312P | P | 20020614 | | |
| | EP 2002-13675 | A | 20020620 | | |
| | WO 2003-EP6016 | W | 20030607 | | |
| OS | MARPAT 140:59654 | | | | |
| AB | Pyrimidinediamines I [R1-R3 = (un)substituted mono- or bicyclic aromatic; R4, R5 = H, Me; A1, A2 = alkylene, CH2CH2O] were prepared for use as protein kinase C θ inhibitors. Thus, 4-amino-1-benzylpiperidine was treated with 5-bromo-2,4-dichloropyrimidine, followed by 2-aminomethylpyridine to give {5-bromo-2-[(2-pyridylmethyl)amino]pyrimidin-4-yl}(1-benzyl-4-piperidinyl)amine which was treated with 3-thiopheneboronic acid to give I [A1, A2 = CH2, R1 = 3-thienyl, R2 = 2-pyridyl, R3 = Ph, R4, R5 = H] which had an IC50 for inhibition of protein kinase C θ < 4.0 μ M. | | | | |
| IT | 637356-54-8P 637356-68-4P 637356-72-0P 637356-78-6P 637356-79-7P 637356-80-0P 637356-81-1P 637356-82-2P 637356-83-3P 637356-84-4P 637356-85-5P 637356-86-6P 637356-87-7P 637356-89-9P 637356-90-2P 637356-91-3P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of substituted diaminopyrimidines as protein kinase C θ inhibitors) | | | | |
| RN | 637356-54-8 CAPLUS | | | | |
| CN | 2,4-Pyrimidinediamine, N4-[1-(phenylmethyl)-4-piperidinyl]-N2-(2-pyridinylmethyl)-5-(3-thienyl)- (9CI) (CA INDEX NAME) | | | | |



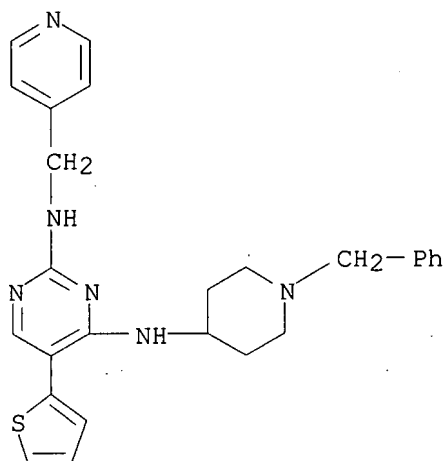
RN 637356-68-4 CAPLUS

CN Benzamide, 4-[[4-[[1-(phenylmethyl)-4-piperidinyl]amino]-2-[(4-pyridinylmethyl)amino]-5-pyrimidinyl]- (9CI) (CA INDEX NAME)



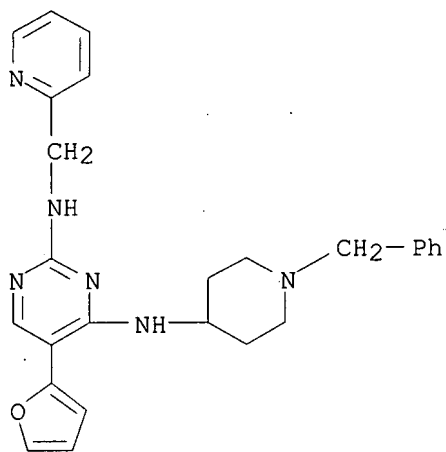
RN 637356-72-0 CAPLUS

CN 2,4-Pyrimidinediamine, N4-[1-(phenylmethyl)-4-piperidinyl]-N2-(4-pyridinylmethyl)-5-(2-thienyl)- (9CI) (CA INDEX NAME)



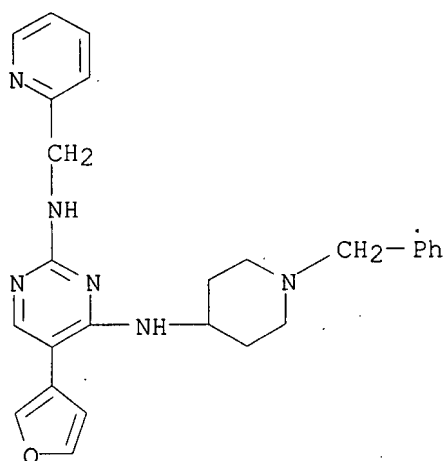
RN 637356-78-6 CAPLUS

CN 2,4-Pyrimidinediamine, 5-(2-furanylmethyl)-N4-[1-(phenylmethyl)-4-piperidinyl]-
N2-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



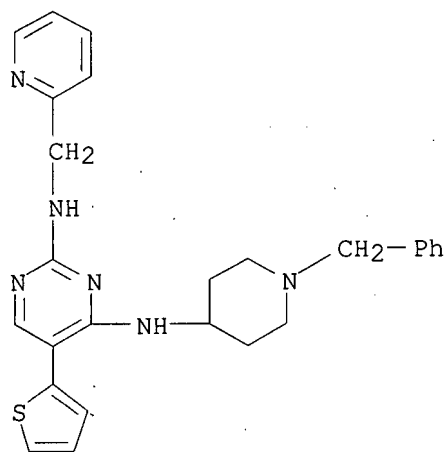
RN 637356-79-7 CAPLUS

CN 2,4-Pyrimidinediamine, 5-(3-furanylmethyl)-N4-[1-(phenylmethyl)-4-piperidinyl]-
N2-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



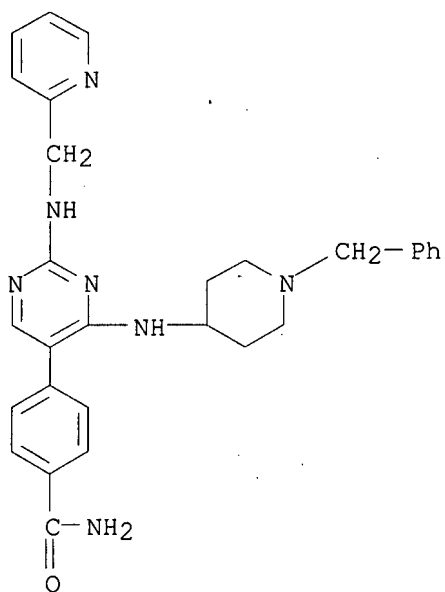
RN 637356-80-0 CAPLUS

CN 2,4-Pyrimidinediamine, N4-[1-(phenylmethyl)-4-piperidinyl]-N2-(2-pyridinylmethyl)-5-(2-thienyl)- (9CI) (CA INDEX NAME)



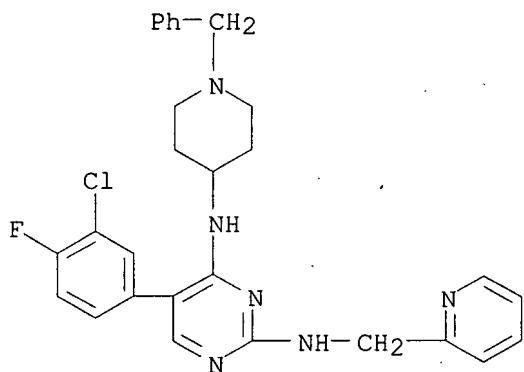
RN 637356-81-1 CAPLUS

CN Benzamide, 4-[4-[[1-(phenylmethyl)-4-piperidinyl]amino]-2-[(2-pyridinylmethyl)amino]-5-pyrimidinyl]- (9CI) (CA INDEX NAME)



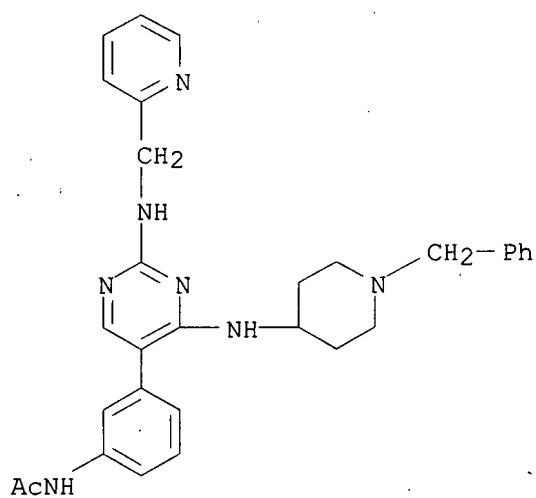
RN 637356-82-2 CAPLUS

CN 2,4-Pyrimidinediamine, 5-(3-chloro-4-fluorophenyl)-N4-[1-(phenylmethyl)-4-piperidinyl]-N2-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



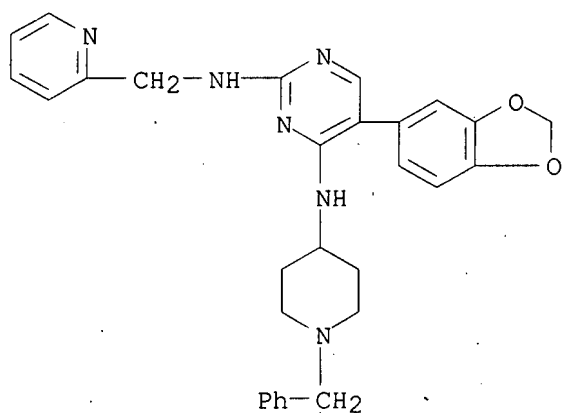
RN 637356-83-3 CAPLUS

CN Acetamide, N-[3-[4-[[1-(phenylmethyl)-4-piperidinyl]amino]-2-[(2-pyridinylmethyl)amino]-5-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)



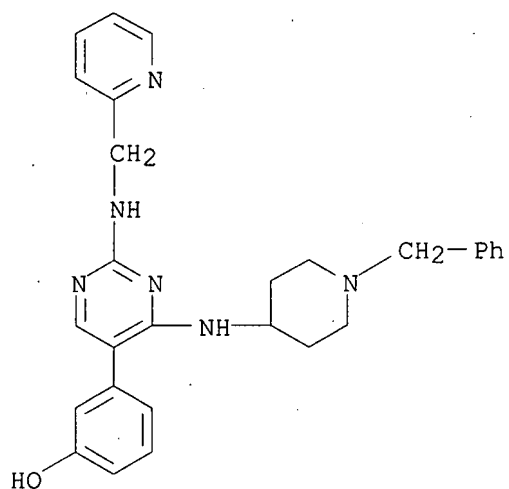
RN 637356-84-4 CAPLUS

CN 2,4-Pyrimidinediamine, 5-(1,3-benzodioxol-5-yl)-N4-[1-(phenylmethyl)-4-piperidinyl]-N2-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



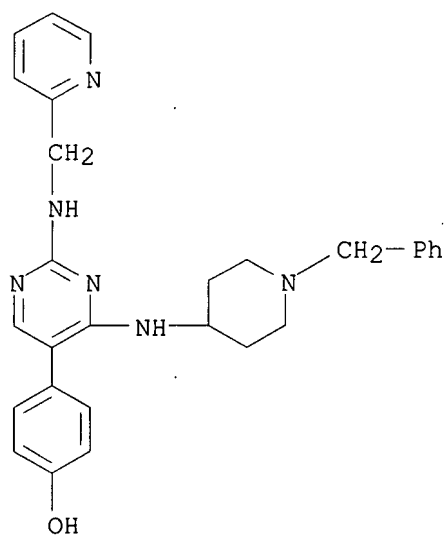
RN 637356-85-5 CAPLUS

CN Phenol, 3-[4-[[1-(phenylmethyl)-4-piperidinyl]amino]-2-[(2-pyridinylmethyl)amino]-5-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 637356-86-6 CAPLUS

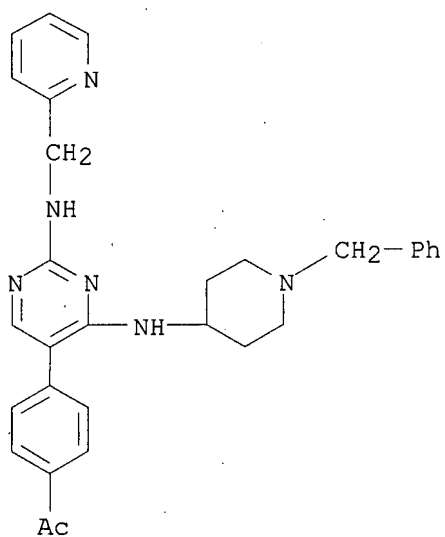
CN Phenol, 4-[4-[[1-(phenylmethyl)-4-piperidinyl]amino]-2-[(2-pyridinylmethyl)amino]-5-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 637356-87-7 CAPLUS

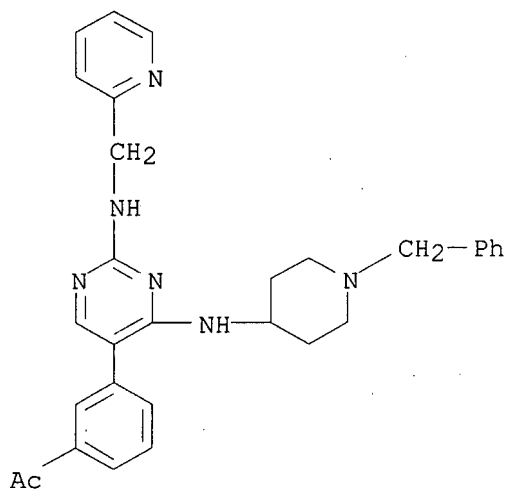
CN Ethanone, 1-[4-[4-[[1-(phenylmethyl)-4-piperidinyl]amino]-2-[(2-pyridinylmethyl)amino]-5-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)

10/517,594



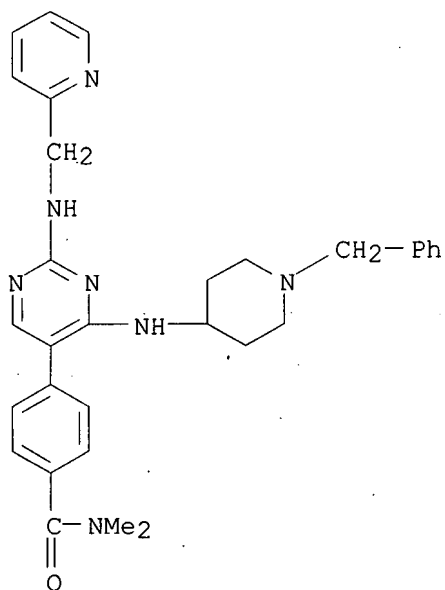
RN 637356-89-9 CAPLUS

CN Ethanone, 1-[3-[4-[[1-(phenylmethyl)-4-piperidinyl]amino]-2-[(2-pyridinylmethyl)amino]-5-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)



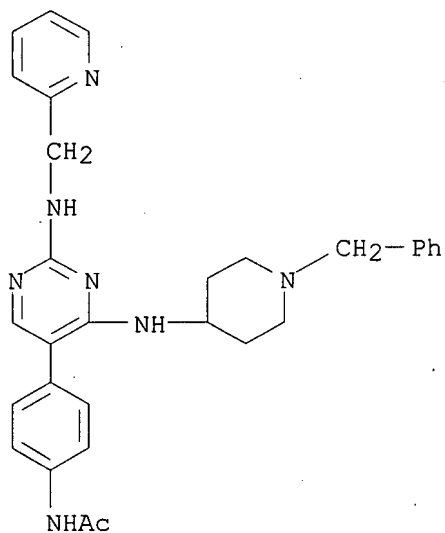
RN 637356-90-2 CAPLUS

CN Benzamide, N,N-dimethyl-4-[4-[[1-(phenylmethyl)-4-piperidinyl]amino]-2-[(2-pyridinylmethyl)amino]-5-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 637356-91-3 CAPLUS

CN Acetamide, N-[4-[4-[[1-(phenylmethyl)-4-piperidinyl]amino]-2-[(2-pyridinylmethyl)amino]-5-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)



IT 637356-57-1P 637356-60-6P 637356-63-9P

637356-66-2P 637356-70-8P 637356-74-2P

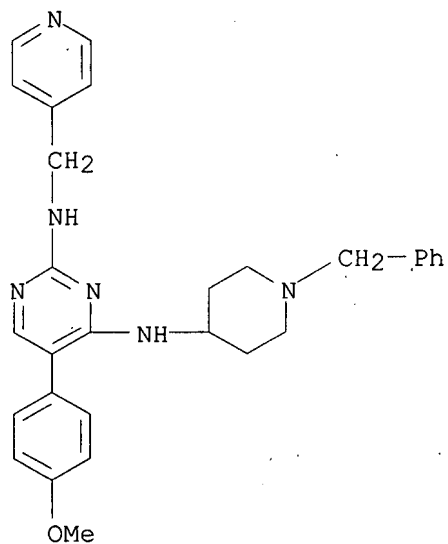
637356-75-3P 637356-76-4P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted diaminopyrimidines as protein kinase C θ inhibitors)

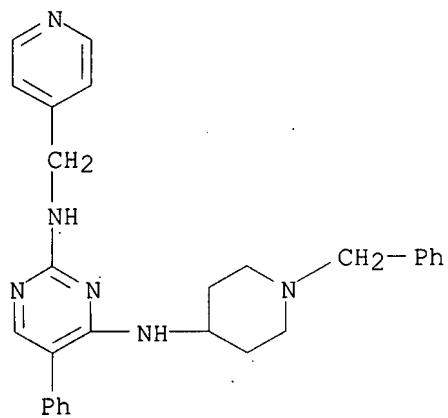
RN 637356-57-1 CAPLUS

CN 2,4-Pyrimidinediamine, 5-(4-methoxyphenyl)-N4-[1-(phenylmethyl)-4-piperidinyl]-N2-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



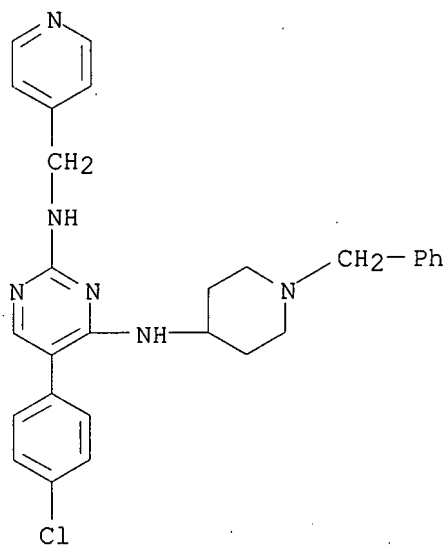
RN 637356-60-6 CAPLUS

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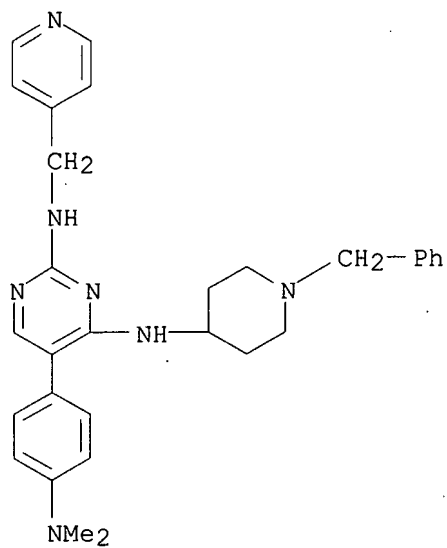
RN 637356-63-9 CAPLUS

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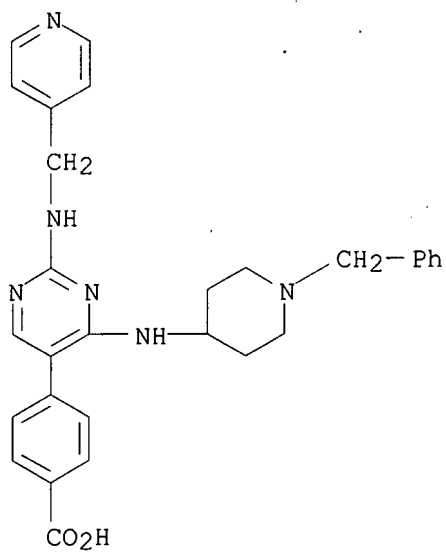
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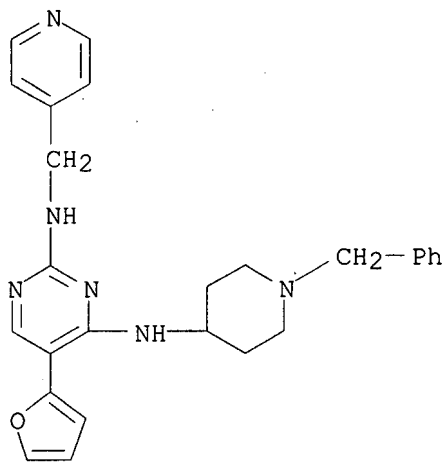
RN 637356-70-8 CAPLUS

CN Benzoic acid, 4-[4-[[1-(phenylmethyl)-4-piperidinyl]amino]-2-[(4-pyridinylmethyl)amino]-5-pyrimidinyl]- (9CI) (CA INDEX NAME)



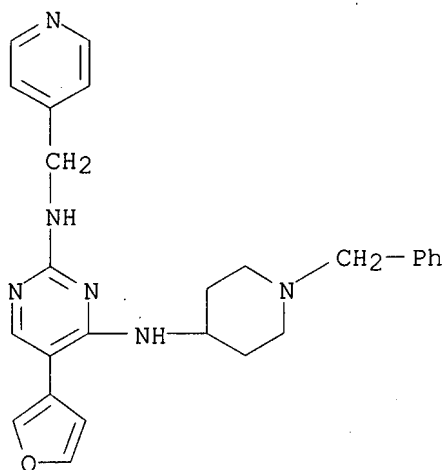
RN 637356-74-2 CAPLUS

CN 2,4-Pyrimidinediamine, 5-(2-furanyl)-N4-[1-(phenylmethyl)-4-piperidinyl]-
N2-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



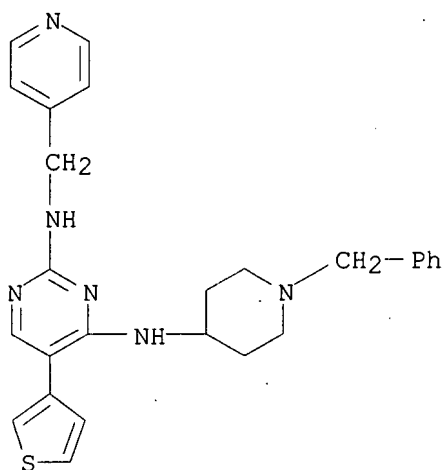
RN 637356-75-3 CAPLUS

CN 2,4-Pyrimidinediamine, 5-(3-furanyl)-N4-[1-(phenylmethyl)-4-piperidinyl]-
N2-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



RN 637356-76-4 CAPLUS

CN 2,4-Pyrimidinediamine, N4-[1-(phenylmethyl)-4-piperidinyl]-N2-(4-pyridinylmethyl)-5-(3-thienyl)- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> log y

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

5.74

178.50

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

ENTRY

TOTAL

SESSION

CA SUBSCRIBER PRICE

-0.78

-0.78

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